547,944

(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization
International Bureau

(43) International Publication Date
16 September 2004 (16.09.2004)

PCT

(10) International Publication Number
WO 2004/079625 A2

(51) International Patent Classification[7]: G06F 19/00

(21) International Application Number:
PCT/DK2004/000148

(22) International Filing Date: 5 March 2004 (05.03.2004)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
PA 2003 00353 7 March 2003 (07.03.2003) DK

(71) Applicant *(for all designated States except US)*: **7TM PHARMA A/S** [DK/DK]; Fremtidsvej 3, DK-2970 Hørsholm (DK).

(72) Inventors; and

(75) Inventors/Applicants *(for US only)*: **FRIMURER, Thomas, Michael** [DK/DK]; Amager Boulevard 130, 4. th., DK-2300 Copenhagen S (DK). **ULVEN, Trond** [SE/DK]; Niels Brocks Gade 6, DK-1574 Copenhagen K (DK). **HÖGBER, Thomas** [SE/SE]; Kabbarpsvägen 6, SE-232 52 Åkarp (SE). **ELLING, Christian, E.** [DK/DK]; Fredensvej 45, DK-2970 Hørsholm (DK).

(74) Agent: **ALBIHNS A/S**; H.C. Andersens Boulevard 49, DK-1553 Copenhagen_V (DK).

(81) Designated States *(unless otherwise indicated, for every kind of national protection available)*: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW.

(84) Designated States *(unless otherwise indicated, for every kind of regional protection available)*: ARIPO (BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

Published:
— *without international search report and to be republished upon receipt of that report*

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

WO 2004/079625 A2

(54) Title: A PSEUDO-SEQUENCE METHOD FOR COMPARING 7TM RECEPTORS WITH RESPECT TO THE PHYSICOCHEMICAL PROPERTIES OF THEIR BINDING SITES

(57) Abstract: A pseudo-sequence method for comparing 7TM receptors with respect to the physicochemical properties of their binding sites, the method comprising the steps of: (i) optionally, aligning part of or all of the amino acid sequence of the first 7TM receptor with part of or all or the amino acid sequence of the one or more further 7TM receptors, (ii) selecting, in a sequential or non-sequential order, at the most 12 amino acid residues per helix and/or extracellular loops, which are involved in one or more binding sites of each 7TM receptor. (iii) forming a pseudo-sequence comprising at the most 50 amino acid residues from the selected sequential or non-sequential amino acid residues, (iv) for each 7TM receptor assigning one or more physicochemical descriptors to the amino acid residues of the selected amino acid pseudo-sequence involved in one or more binding sites, (v) optionally, for each 7TM receptor mathematically manipulating the physicochemical descriptors of step (iv) to obtain a simplified measure of the physicochemical properties of the binding site. (vi) for each 7TM receptor generating a similarity score as defined herein by comparing the physicochemical descriptor or, if relevant, the simplified measure for the first 7TM receptor with the physicochemical descriptors or, if relevant, the simplified measures for the one or further 7TM receptors, (vii) optionally, ranking the 7TM receptors with respect to the physicochemical properties of their binding sites according to the similarity scores obtained in step vi)